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14. ABSTRACT The current work focuses on evaluation of the effective elastic properties of cementitious materials through a voxel based FEA approach. Voxels are generated for a heterogeneous cementitious material (Type-I cement) consisting of typical volume fractions of various constituent phases from digital microstructures. The microstructure is modeled as a micro-scale representative volume element (RVE) in ABAQUS to generate cubes several tens of microns in dimension and subjected to various prescribed deformation modes to generate the effective elastic tensor of the material. The RVE calculated elastic properties such as moduli and Poisson's ratio are validated through an					
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Report Title

Micromechanics Based Representative Volume Element Modeling of Heterogeneous Cement Paste

ABSTRACT

The current work focuses on evaluation of the effective elastic properties of cementitious materials through a voxel based FEA approach. Voxels are generated for a heterogeneous cementitious material (Type-I cement) consisting of typical volume fractions of various constituent phases from digital microstructures. The microstructure is modeled as a micro-scale representative volume element (RVE) in ABAQUS to generate cubes several tens of microns in dimension and subjected to various prescribed deformation modes to generate the effective elastic tensor of the material. The RVE-calculated elastic properties such as moduli and Poisson's ratio are validated through an asymptotic expansion homogenization (AEH) and compared with rule of mixtures. Both Periodic (PBC) and Kinematic boundary conditions (KBC) are investigated to determine if the elastic properties are invariant due to boundary conditions. In addition the method of "Windowing" was used to assess the randomness of the constituents and to validate how the isotropic elastic properties were determined. The average elastic properties obtained from the displacement based FEA of various locally anisotropic micro-size cubes extracted from an RVE of size 100x100x100 microns showed that the overall RVE response was fully isotropic. The effects of domain size, degree of hydration, kinematic and periodic boundary conditions, domain sampling techniques, local anisotropy, particle size distribution (PSD), and random microstructure on elastic properties are studied.



Multi-Scale Modeling of Cementitious Materials



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Abstract

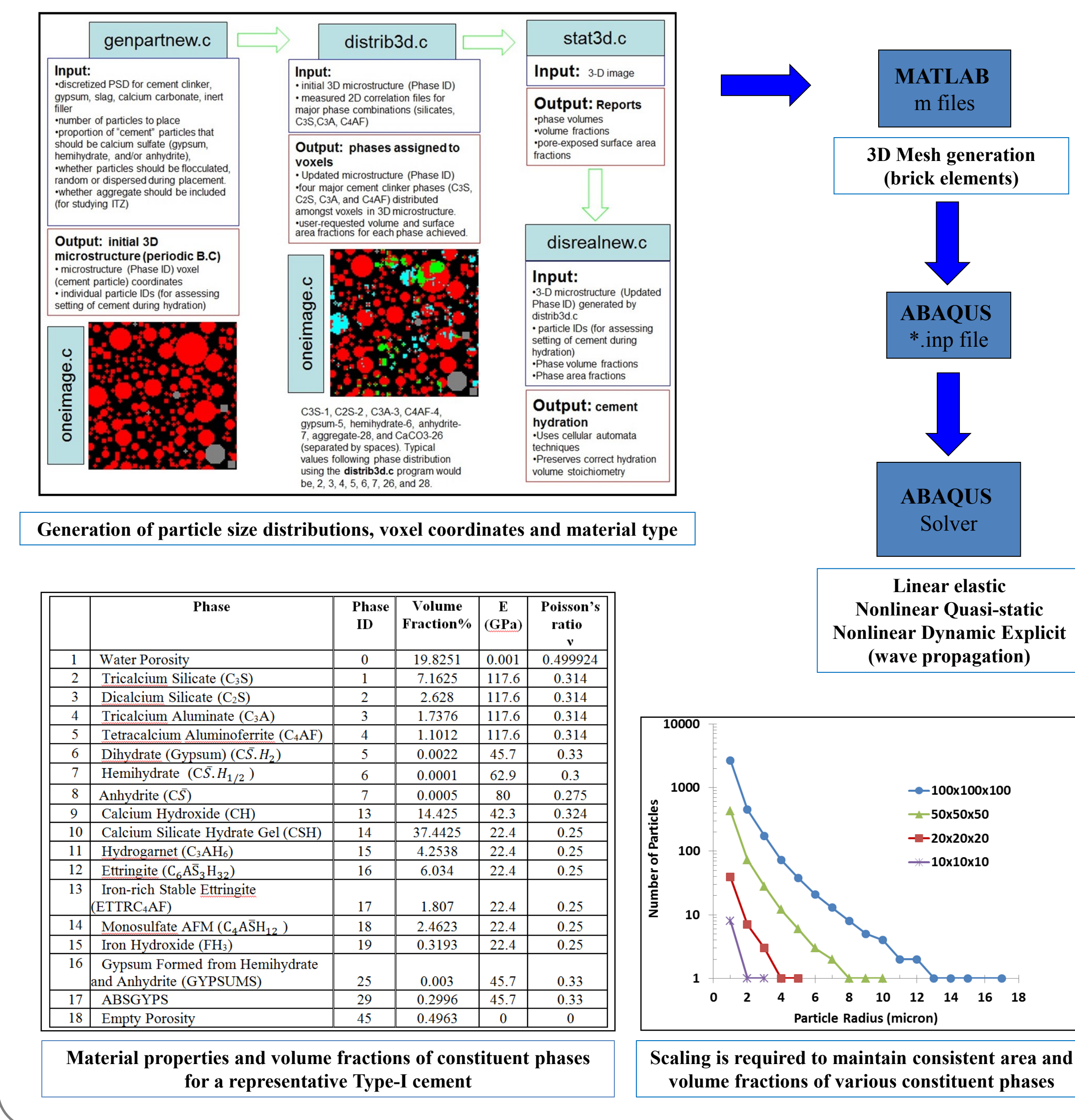
- Effective elastic properties of cementitious materials are evaluated through a voxel based FEA approach.

Introduction

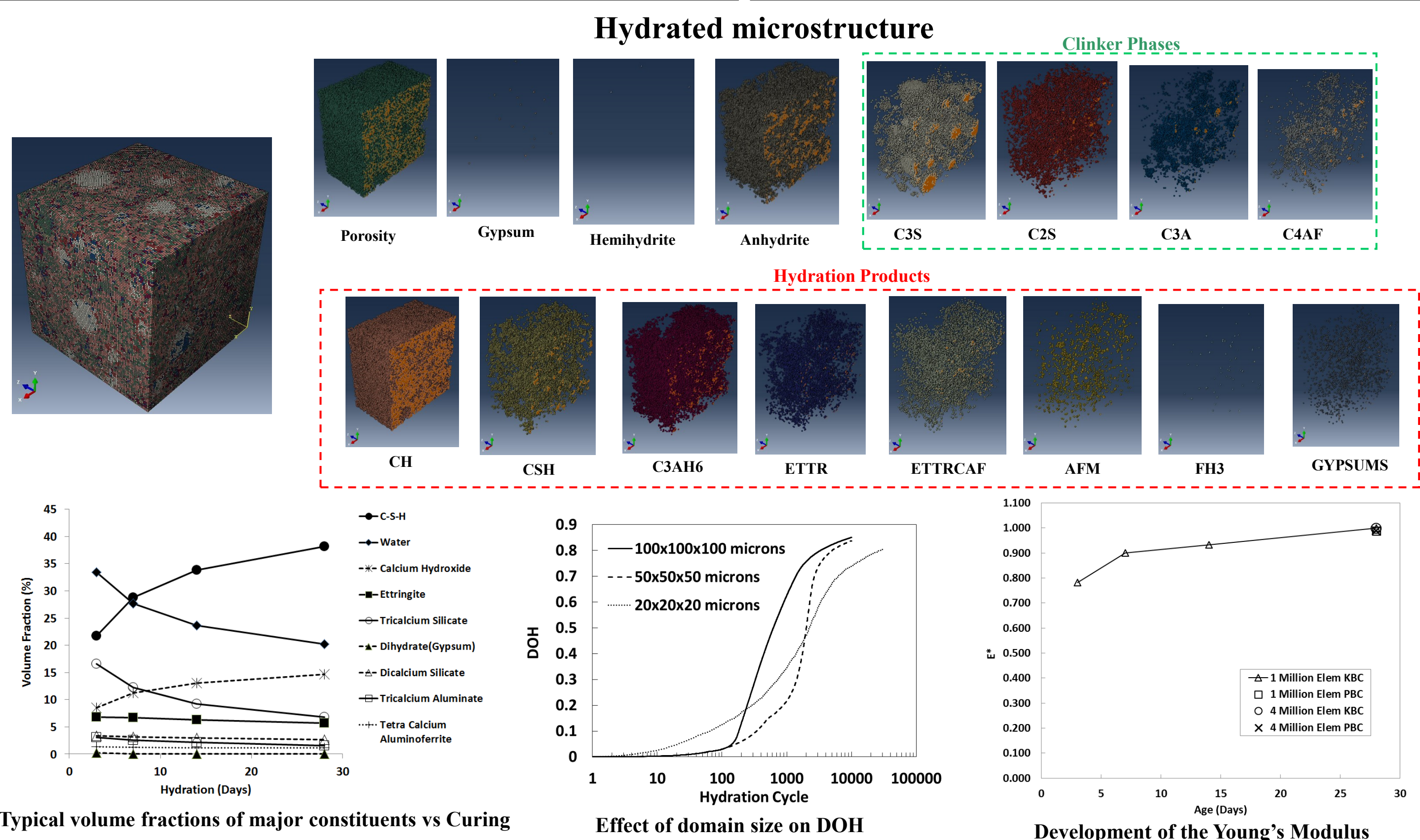
- A methodology has been developed for computing the elastic properties of heterogeneous C-S-H (calcium oxide- silicate oxide- hydroxide) based multi-phase cementitious materials.
- The primary focus is to predict homogenized properties at macro-levels using micro mechanics based models.
- Focus is on the determination of elastic properties for hydrated cement paste from un-hydrated constituents when small strain quasi-static loading conditions are applied to micro-scale.

Methodology

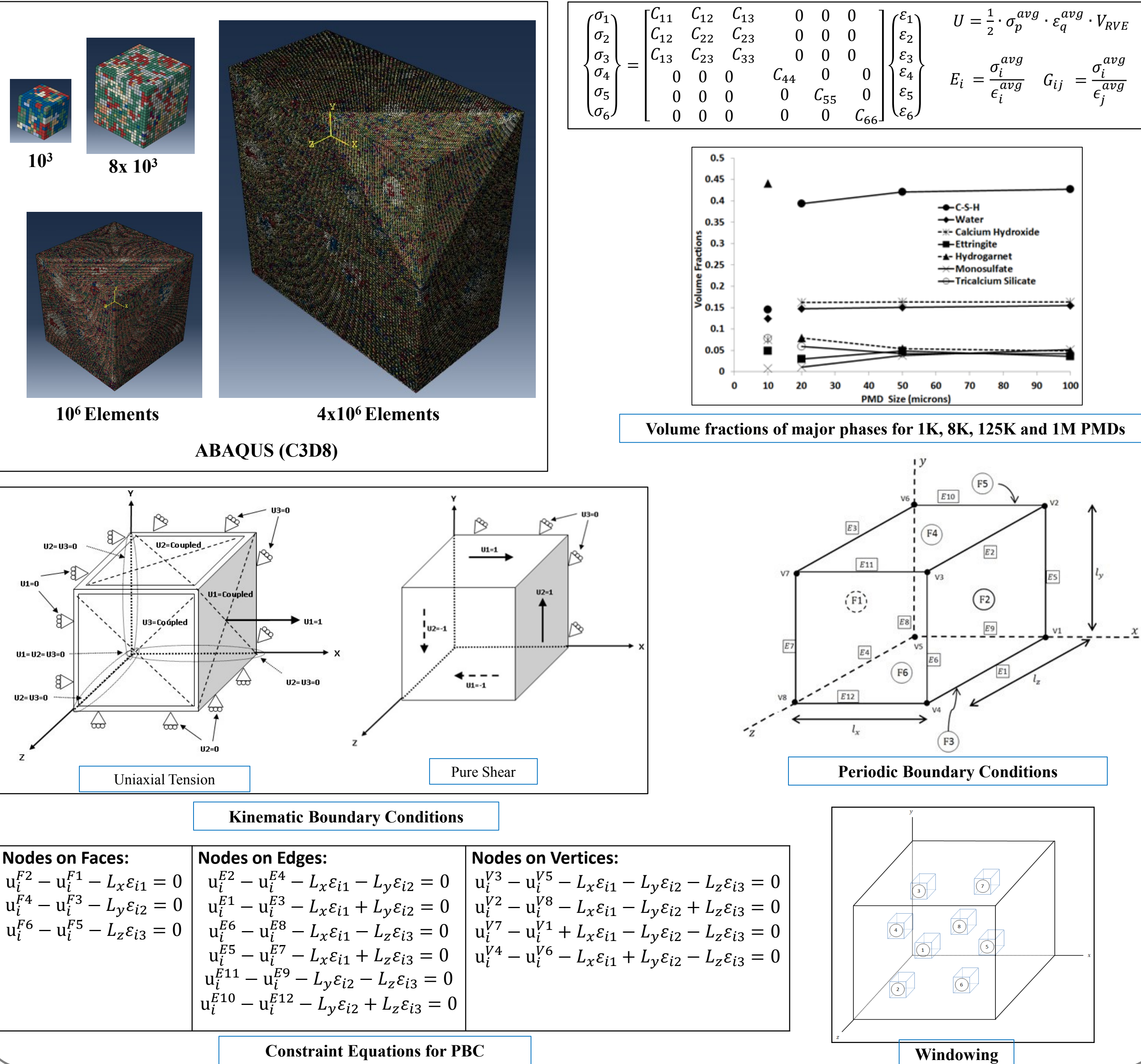
- The representative volume element (RVE) is the smallest volume of material that captures global characteristics of the material and shows the same overall material properties irrespective of the boundary conditions applied.
- Software package CEMHYD3D V.3 (NIST), simulates the hydration process and formation of the digitally generated micro-structure for a typical Type-I general purpose cement.
- Initial 3D microstructure is created based on measured geometrical particle size distribution (PSD) as well as volume fractions and surface-area fractions of the constituent phases for cement powder, extracted from 2D composite images of cement at various degrees of hydration (DOH).
- The RVE-calculated elastic properties such as moduli and Poisson's ratio are validated through an asymptotic expansion homogenization (AEH) and compared with rule of mixtures.
- Windowing is employed to investigate how anisotropy due to local microstructure leads to overall isotropic behavior of the agglomerate. Windows are analogous to physical core samples prepared by extraction from a hydrated bulk specimen.



Cement Hydration



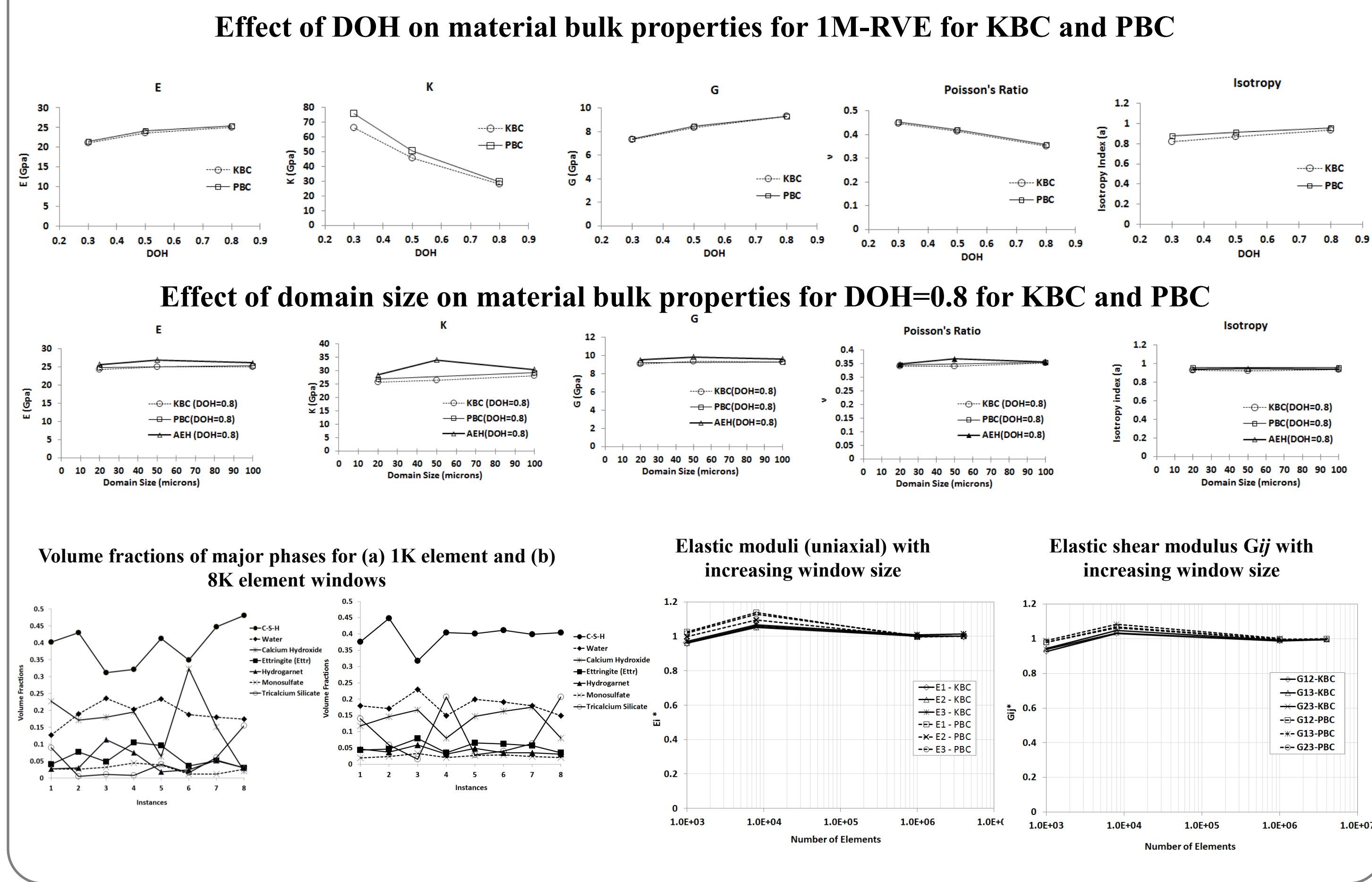
RVE



AEH

- Subject to PBC, exact estimate of the effective homogeneous elastic properties can be obtained for linear elastic inhomogeneous microstructures that exhibit perfectly-periodic homogeneity by solving for χ_k^{mn} in:
- Vector y_i signifies the coordinates of the microstructure RVE, and D_{ijk} is the elastic stiffness tensor at a point y in the material. The homogenized linear elastic stiffness tensor, D_{ijmn}^{hom} is given:

Microstructure Based Homogenization



Rule of Mixtures Based Homogenization

- A rule of mixtures approach independent of the microstructure of the material is used to compute the effective bulk properties of the cementitious material.
 - The theoretical extreme upper and lower bounds on effective material properties of multi-phase materials are the Voigt (1928) and Reuss (1929) bounds.
- $$K^* = \sum_{i=1}^n f_i K_i \quad G^* = \sum_{i=1}^n f_i G_i$$
- $$\frac{1}{K^*} = \sum_{i=1}^n \frac{f_i}{K_i} \quad \frac{1}{G^*} = \sum_{i=1}^n \frac{f_i}{G_i}$$
- Hashin(1962) presented the composite (or coated) spheres model for determining the effective material properties for multi-phase materials, based on the dilute suspension model.
- $$\frac{K^*}{K_m} = 1 + 3(1 - v_m) \sum_{i=1}^n \frac{\left(\frac{K_i}{K_m} - 1\right) c_i}{2(1 - 2v_m) + (1 + v_m) \left[\frac{K_i}{K_m} - \left(\frac{K_i}{K_m} - 1\right) c\right]}$$
- $$\frac{G^*}{G_m} = 1 + 15(1 - v_m) \sum_{i=1}^n \frac{\left(\frac{G_i}{G_m} - 1\right) c_i}{7 - 5v_m + 2(4 - 5v_m) \frac{G_i}{G_m} - 2(4 - 5v_m) \left(\frac{G_i}{G_m} - 1\right) c}$$
- For Hashin and Voigt estimates, the bulk modulus (K) is found to be lower compared to the values computed based on the microstructure (KBC, PBC and AEH). Both the Young's Modulus (E) and shear modulus (G) are determined to be higher than those estimated by microstructure based homogenization.

Conclusion

- A comparison between the two domain sampling methods shows that windowing produces effective material properties with a larger variation than the PMD due to a higher variation in local phase volume fractions.
- Macroscopic properties obtained for various DOH and domain sizes, determined by applying Kinematic Boundary Conditions (KBC), Periodic Boundary Conditions (PBC), AEH and rule of mixtures based homogenization are found to be comparable.
- It is shown that even though cement is a heterogeneous anisotropic material at the micro-level, the bulk properties are effectively isotropic.

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